Calculations

11.2.2.3 recall and understand the use of the ‘molar volume’

11.2.2.4 recall and be able to use the ideal gas equation

11.2.2.7 understand the purpose of, be able to carry out, and be able to carry out calculations involving, titration

11.1.1.7 be able to calculate empirical and molecular formulas from analysis data

11.2.2.8 be able to calculate theoretical yield and percentage yield of reactions

11.2.2.9 understand and be able to calculate atom economy

The ideal gas equation

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Room temperature and pressure, RTP

Limitations

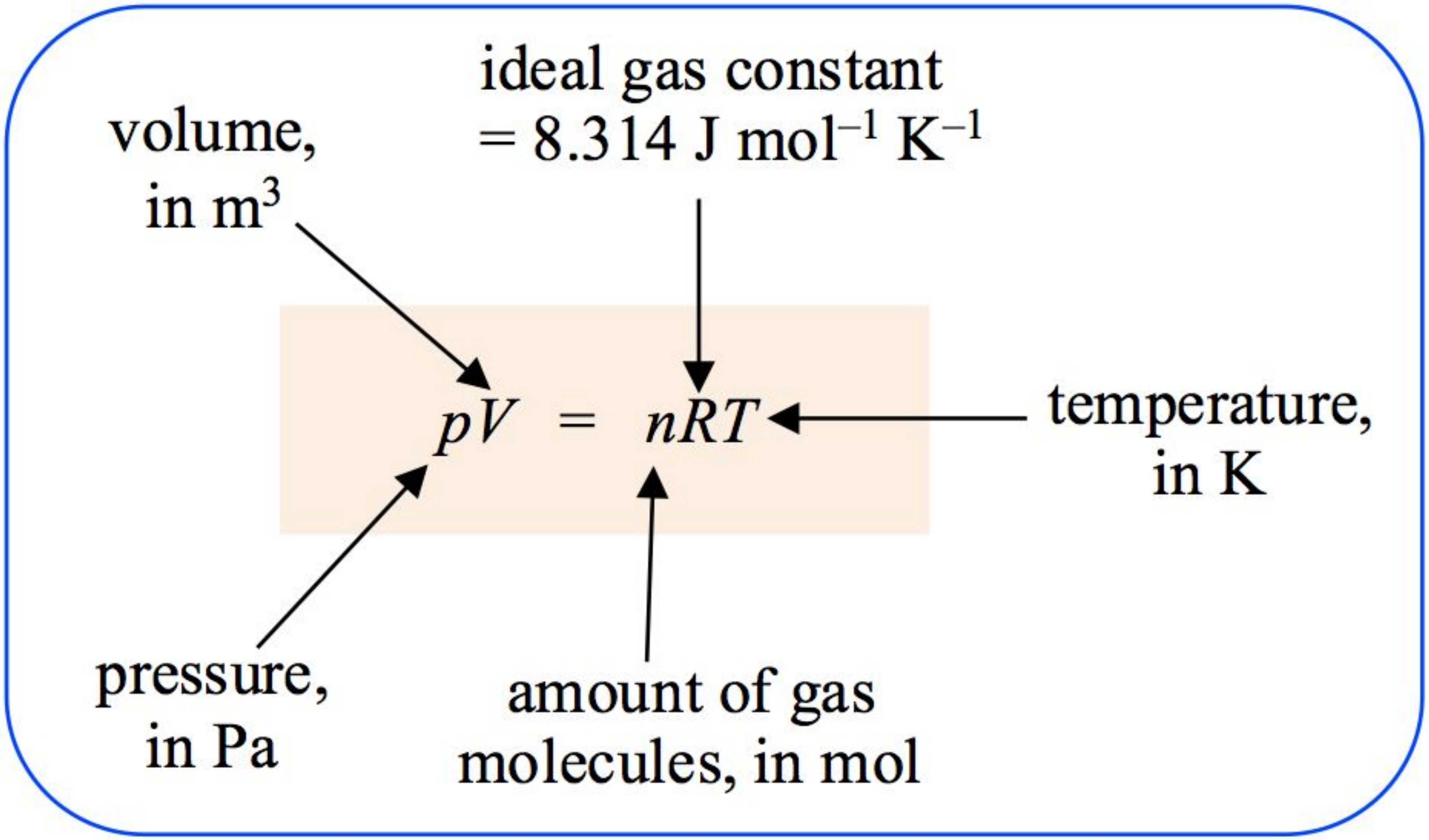
- At RTP, 1 mol of gas molecules occupies 24.0 dm^3
- Conditions are not always room temperature and pressure.
- A gas volume depends on temperature and pressure.

Ideal gas equation can calculate a gas volume, V

- at any temperature, T
- at any pressure, p

The ideal gas equation

$$pV = nRT$$



Converting units for $pV = nRT$

Before using $pV = nRT$, convert units to m^3, K and Pa

- cm^3 to m^3 $\times 10^{-6}$
- dm^3 to m^3 $\times 10^{-3}$
- °C to K $+ 273$
- kPa to Pa $\times 10^3$

Examples

- 220 cm^3 = 220 $\times 10^{-6}$ cm^3
- 4.0 dm^3 = 4.0 $\times 10^{-3}$ m^3
- 48 °C = 48 + 273 = 321 K
- 100 kPa = 100 $\times 10^3$ Pa

Calculating gas volumes

Calculate the volume of 0.125 mol of $O_2(g)$ at 75 ºC and 250 kPa

Convert units

75 ºC = 75 + 273 K = 348 K

250 kPa = 250×10^3 Pa

Find the volume, *V*, from the ideal gas equation

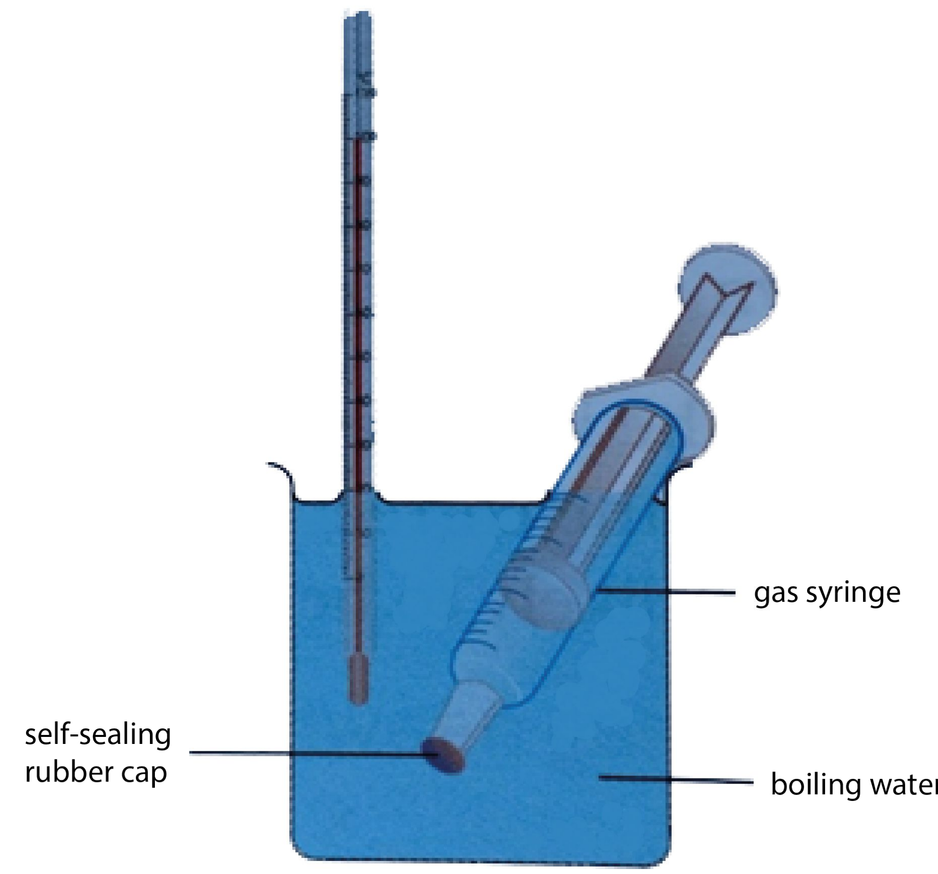
$$pV = nRT$$

$$V = \frac{nRT}{p} = \frac{0.125 \times 8.314 \times 348}{250 \times 10^3}$$

$$\therefore V = 1.45 \times 10^{-3}\ \text{m}^3 = 1.45\ \text{dm}^3$$

Calculating a relative molecular mass

Calculate the volume of 0.125 mol of O_2(g) at 75 ºC and 250 kPa



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Ideal Gas Law

What is the volume that 500 g of iodine will occupy under the conditions: Temp = 300°C and Pressure = 740 mm Hg?

Step 1) Write down given information.

mass = 500 g iodine

$n = 1.9685$ mol I_2

$T = 573$ K (300°C)

$P = 0.9737$ atm (740 mm Hg)

$R = 0.0821$ atm · L / mol · K

$V = ?$ L

Step 2) Equation: $PV = nRT$

Step 3) Solve for variable

$$V = \frac{nRT}{P}$$

Step 4) Substitute in numbers and solve

$$V = \frac{(1.9685 \text{ mol})(0.0821 \text{ atm} \cdot \text{L / mol} \cdot \text{K})(573 \text{ K})}{0.9737 \text{ atm}}$$

$$V = 95.1 \text{ L } I_2$$

AN INTRODUCTION TO

ATOM ECONOMY

KNOCKHARDY PUBLISHING

ATOM ECONOMY

In most reactions you only want to make one of the resulting products

Atom economy is a measure of how much of the products are useful

A high atom economy means that there is less waste

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ATOM ECONOMY

$$\frac{\text{MOLECULAR MASS OF DESIRED PRODUCT}}{\text{SUM OF MOLECULAR MASSES OF ALL PRODUCTS}} \times 100$$

2015 A level

Example 1

WORKED CALCULATIONS

Calculate the atom economy for the formation of 1,2-dichloroethane, $C_2H_4Cl_2$

Example 1

ORKED CALCULATIONS

Calculate the atom economy for the formation of 1,2-dichloroethane, $C_2H_4Cl_2$

Equation	C_2H_4	+	Cl_2	$\longrightarrow$	$C_2H_4Cl_2$
M_r	28		71		99

$$\text{atom economy} = \frac{\text{molecular mass of } C_2H_4Cl_2}{\text{molecular mass of all products}} \times 100$$

$$= \frac{99}{99} \times 100 = \underline{100\%}$$

An ATOM ECONOMY of 100% is typical of an ADDITION REACTION

Example 2

ORKED CALCULATIONS

Calculate the atom economy for the formation of nitrobenzene, $C_6H_5NO_2$

Example 2

WORKED CALCULATIONS

Calculate the atom economy for the formation of nitrobenzene, $C_6H_5NO_2$

Equation	C_6H_6	+	HNO_3	$\longrightarrow$	$C_6H_5NO_2$	+	H_2O
M_r	78		63		123		18

$$\text{atom economy} = \frac{\text{molecular mass of } C_6H_5NO_2}{\text{molecular mass of all products}} \times 100$$

$$= \frac{123}{123 + 18} \times 100 = \underline{87.2\%}$$

An ATOM ECONOMY of 100% is not possible with a SUBSTITUTION REACTION

Example 3

WORKED CALCULATIONS

Calculate the atom economy for the preparation of ammonia from the thermal decomposition of ammonium sulphate.

Example 3

ORKED CALCULATIONS

Calculate the atom economy for the preparation of ammonia from the thermal decomposition of ammonium sulphate.

Equation $(NH_4)_2SO_4 \longrightarrow H_2SO_4 + 2NH_3$

M_r 132 98 17

$$\text{atom economy} = \frac{2 \text{ x molecular mass of } NH_3}{\text{molecular mass of all products}} \text{ x } 100$$

$$= \frac{2 \text{ x } 17}{98 + (2 \text{ x } 17)} = 25.8\%$$

In industry a low ATOM ECONOMY isn't necessarily that bad if you can use some of the other products. If this reaction was used industrially, which it isn't, the sulphuric acid would be a very useful by-product.

CALCULATIONS

Calculate the atom economy of the following reactions (the required product is shown in red)

- CH_3COCl + $C_2H_5NH_2$ ——> $CH_3CONHC_2H_5$ + HCl
- C_2H_5Cl + $NaOH$ ——> C_2H_5OH + $NaCl$
- C_2H_5Cl + $NaOH$ ——> C_2H_4 + H_2O + $NaCl$

CALCULATIONS

Calculate the atom economy of the following reactions (the required product is shown in red)

- CH_3COCl + $C_2H_5NH_2$ ——> $CH_3CONHC_2H_5$ + HCl

70.2 %

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CALCULATIONS

Calculate the atom economy of the following reactions (the required product is shown in red)

- CH_3COCl + $C_2H_5NH_2$ ——> $CH_3CONHC_2H_5$ + HCl — 70.2 %
- C_2H_5Cl + $NaOH$ ——> C_2H_5OH + $NaCl$ — 55.8 %
- C_2H_5Cl + $NaOH$ ——> C_2H_4 + H_2O + $NaCl$ — 33.9 %

OVERVIEW

- addition reactions will have 100% atom economy

- substitution reactions will have less than 100% atom economy

- high atom economy = fewer waste materials
  = GREENER and MORE ECONOMICAL

The percentage yield of a reaction must also be taken into consideration.

- some reactions may have a high yield but a low atom economy
- some reactions may have a high atom economy but a low yield

Reactions involving equilibria must also be considered

Percentage yield

Perform calculations to determine the **percentage yield** of a reaction

In a chemical reaction which is totally efficient all the REACTANTS are converted into products.
This will give 100% yield.
Most reactions, particularly organic reactions give low yields.
Possible reasons:
Impure reactants.
Product is lost during purification.
Side reactions.
Equilibrium reaction means that a reaction is never completed.

Definitions

- Know that:
- **The theoretical yield** is the maximum mass of products which would be obtained from the balanced equation.
- **The actual yield** is the mass of products obtained.

- The percentage yield = $\dfrac{\text{Actual yield}}{\text{Theoretical yield}} \times 100\%$

- **Limiting reactant** is the substance present in lowest quantity which determines the actual yield.
- Excess – more than the mass determined by the balanced equation is used to maximise product obtained.

Calculating Percentage (%) Yield

2.3g of sodium reacts with an excess of chlorine to produce 4.0g of sodium chloride.

What is the percentage yield?

$$2Na_{(s)} \quad + \quad Cl_{2(g)} \quad \Rightarrow \quad 2NaCl_{(s)}$$

(A_r reactants: Na=23 Cl=35.5 M_r product: NaCl= 58.5)

$$2.3g\ Na = \frac{2.3}{23}\ mol\ Na \quad = 0.1\ mol\ Na$$

Theoretically 0.1 mol Na should yield 0.1 mol NaCl

Theoretical yield of NaCl = 58.5 x 0.1 = 5.85g

$$\%\ Yield = \frac{\text{Actual yield}}{\text{Theoretical yield}} \times 100\% \qquad \%\ Yield = \frac{4.0g}{5.85g} \times 100\% = 68\%$$

Calculating Percentage (%) Yield

If 1.2g of magnesium reacts with an excess of oxygen to produce 0.8g of magnesium oxide…

What is the percentage yield?

$$2Mg_{(s)} + O_{2(g)} \Rightarrow 2MgO_{(s)}$$

(A_r reactants: Mg=24 O=16 M_r product: MgO= 40)

$$1.2g\ Mg = \frac{1.2}{24}\ mol\ Mg = 0.05\ mol\ Mg$$

Theoretically 0.05 mol Mg should yield 0.05 mol MgO

Theoretical yield of MgO = 40 x 0.05 = 2g

$$\%\ Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% \qquad \%\ Yield = \frac{0.8g}{2g} \times 100\% = 40\%$$

Calculating Percentage (%) Yield

If 2g of calcium carbonate reacts with an excess of hydrochloric acid to produce 1.11 g of calcium chloride….

What is the percentage yield?

$$2HCl_{(aq)} + CaCO_{3(s)} \Rightarrow H_2O_{(l)} + CO_{2(g)} + CaCl_{2(s)}$$

(M_r values are: $CaCO_3 = 100$ $CaCl_2 = 111$)

$$2g\ CaCO_3 = \frac{2}{100}\ mol\ CaCO_3 = 0.02\ mol\ CaCO_3$$

Theoretically 0.02 mol $CaCO_3$ should yield 0.02 mol $CaCl_2$

Theoretical Yield of $CaCl_2$ = 111 x 0.02 = 2.22g

$$\%\ Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\%$$

$$\%\ Yield = \frac{1.11}{2.22} \times 100 = 50\%$$